Sucralose

56038-13-2 | DTXSID1040245

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: -0.0180

Global applicability domain: Outside

Local applicability domain index: 2.35e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

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Tris(2-hydroxyethyl)
isocyanurate
Measured: 0.2
Predicted: 2.08e-01

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Triisopropanolamine
Measured: -0.240
Predicted: -0.130

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Malaoxon
Measured: 0.05
Predicted: 1.75e-01

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Hexamethylphosphoramide
Measured: -0.300
Predicted: -0.141

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Pentaerythritol
Measured: 0.1
Predicted: 9.76e-02